



README.txt

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I. Introduction:

THIS SOURCE CODE IS NOT TO BE DUPLICATED WITHOUT PERMISSION

This Disk contains the source code (written in the C/C++ programming language)
for US Patent Application of Pang et al. for "A COMPUTATIONAL METHOD FOR PREDICTING
INTRAMOLECULAR AND INTERMOLECULAR BIOPOLYMER INTERACTIONS"

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Filing By: Baker Botts LLP, 30 Rockefeller Plaza, New York, NY, 10112.

II. Files:

The Microsoft Visual C++ 6.0 Programming environment was used:

The workspace file is: Shevek.dsw

The project file is: Shevek.dsp

Source files include:

ApplyThresh.c
ChainElim.c
definitions.h
FASTEXP2.C
FASTEXP2.H
FASTEXP2.INC
GETTIMER.C
MainExactPScore.c
MainMisalign.c
MainScreening.c
MainShevek.c
MisalignNRPang.c
nrutilp.h
NumRecPang.c
NumRecUtilities.c
PRCERR.C
RandNumGen.c
RCONT2p.H
Rcount2Pang.C
shevek.h
SUPPORT.C
SUPPORT.H

Text files include:

degenmsg
eliminatmsg
misalignmsg
predictmsg
scoremsg
threshmsg
titlepage

III. General Program Structure:

FUNCTION	PURPOSE	FOUND IN FILE
main()	[driving function]	MainShevek.c
----- openfile()	[reads alignment]	MainShevek.c
----- score_manager()	[scoring]	MainShevek.c
----- screener()	[screening]	MainScreening.c
----- misalign_identifier()	[misalignment]	MainMisalign.c

```

                                Shevek.dsp
# Microsoft Developer Studio Project File - Name="shev" - Package Owner=<4>
# Microsoft Developer Studio Generated Build File, Format Version 6.00
# ** DO NOT EDIT **

# TARGTYPE "Win32 (x86) Console Application" 0x0103

CFG=shev - Win32 Debug
!MESSAGE This is not a valid makefile. To build this project using NMAKE,
!MESSAGE use the Export Makefile command and run
!MESSAGE
!MESSAGE NMAKE /f "Shevek.mak".
!MESSAGE
!MESSAGE You can specify a configuration when running NMAKE
!MESSAGE by defining the macro CFG on the command line. For example:
!MESSAGE
!MESSAGE NMAKE /f "Shevek.mak" CFG="shev - Win32 Debug"
!MESSAGE
!MESSAGE Possible choices for configuration are:
!MESSAGE
!MESSAGE "shev - Win32 Release" (based on "Win32 (x86) Console Application")
!MESSAGE "shev - Win32 Debug" (based on "Win32 (x86) Console Application")
!MESSAGE

# Begin Project
# PROP AllowPerConfigDependencies 0
# PROP Scc_ProjName ""
# PROP Scc_LocalPath ""
CPP=xicl6.exe
RSC=rc.exe

!IF "$(CFG)" == "shev - Win32 Release"

# PROP BASE Use_MFC 0
# PROP BASE Use_Debug_Libraries 0
# PROP BASE Output_Dir "Release"
# PROP BASE Intermediate_Dir "Release"
# PROP BASE Target_Dir ""
# PROP Use_MFC 0
# PROP Use_Debug_Libraries 0
# PROP Output_Dir "Release"
# PROP Intermediate_Dir "Release"
# PROP Target_Dir ""
# ADD BASE CPP /nologo /W3 /GX /O2 /D "WIN32" /D "NDEBUG" /D "_CONSOLE" /D "_MBCS" /YX /FD /c
# ADD CPP /nologo /W3 /GX /O2 /D "WIN32" /D "NDEBUG" /D "_CONSOLE" /D "_MBCS" /YX /FD /c
# ADD BASE RSC /l 0x409 /d "NDEBUG"
# ADD RSC /l 0x409 /d "NDEBUG"
BSC32=bscmake.exe
# ADD BASE BSC32 /nologo
# ADD BSC32 /nologo
LINK32=xilink6.exe
# ADD BASE LINK32 kernel32.lib user32.lib gdi32.lib winspool.lib comdlg32.lib advapi32.lib
shell32.lib ole32.lib oleaut32.lib uuid.lib odbc32.lib odbccp32.lib /nologo /subsystem:console
/machine:I386
# ADD LINK32 kernel32.lib user32.lib gdi32.lib winspool.lib comdlg32.lib advapi32.lib shell32.lib
ole32.lib oleaut32.lib uuid.lib odbc32.lib odbccp32.lib /nologo /subsystem:console /machine:I386

!ELSEIF "$(CFG)" == "shev - Win32 Debug"

# PROP BASE Use_MFC 0
# PROP BASE Use_Debug_Libraries 1
# PROP BASE Output_Dir "Debug"
# PROP BASE Intermediate_Dir "Debug"
# PROP BASE Target_Dir ""
# PROP Use_MFC 0
# PROP Use_Debug_Libraries 1
# PROP Output_Dir "Debug"
# PROP Intermediate_Dir "Debug"
# PROP Target_Dir ""
# ADD BASE CPP /nologo /W3 /Gm /GX /ZI /Od /D "WIN32" /D "_DEBUG" /D "_CONSOLE" /D "_MBCS" /YX /FD
/GZ /c
# ADD CPP /nologo /W3 /Gm /GX /ZI /Od /D "WIN32" /D "_DEBUG" /D "_CONSOLE" /D "_MBCS" /FR /YX /FD /GZ
/c
# ADD BASE RSC /l 0x409 /d "_DEBUG"
# ADD RSC /l 0x409 /d "_DEBUG"
BSC32=bscmake.exe
# ADD BASE BSC32 /nologo
# ADD BSC32 /nologo
LINK32=xilink6.exe

```

```

                                Shevek.dsp
# ADD BASE LINK32 kernel32.lib user32.lib gdi32.lib winspool.lib comdlg32.lib advapi32.lib
shell32.lib ole32.lib oleaut32.lib uuid.lib odbc32.lib odbccp32.lib /nologo /subsystem:console /debug
/machine:I386 /pdbtype:sept
# ADD LINK32 kernel32.lib user32.lib gdi32.lib winspool.lib comdlg32.lib advapi32.lib shell32.lib
ole32.lib oleaut32.lib uuid.lib odbc32.lib odbccp32.lib /nologo /subsystem:console /debug
/machine:I386 /pdbtype:sept

!ENDIF

# Begin Target

# Name "shev - Win32 Release"
# Name "shev - Win32 Debug"
# Begin Group "Source Files"

# PROP Default_Filter "cpp;c;cxx;rc;def;r;odl;idl;hpj;bat"
# Begin Group "Primary Files"

# PROP Default_Filter ""
# Begin Source File

SOURCE=.\MainShevek.c
# End Source File
# Begin Source File

SOURCE=.\NumRecPang.c
# End Source File
# Begin Source File

SOURCE=.\NumRecUtilities.c
# End Source File
# End Group
# Begin Group "MonteCarloSim"

# PROP Default_Filter ""
# Begin Source File

SOURCE=.\FASTEXP2.C
# End Source File
# Begin Source File

SOURCE=.\FASTEXP2.INC
# End Source File
# Begin Source File

SOURCE=.\GETTIMER.C
# End Source File
# Begin Source File

SOURCE=.\MainExactPScore.c
# End Source File
# Begin Source File

SOURCE=.\PRCERR.C
# End Source File
# Begin Source File

SOURCE=.\RandNumGen.c
# End Source File
# Begin Source File

SOURCE=.\Rcount2Pang.C
# End Source File
# Begin Source File

SOURCE=.\SUPPORT.C
# End Source File
# End Group
# Begin Group "Screening"

# PROP Default_Filter ""
# Begin Source File

SOURCE=.\ApplyThresh.c
# End Source File
# Begin Source File

SOURCE=.\ChainElim.c

```

```
# End Source File
# Begin Source File

SOURCE=.\MainScreening.c
# End Source File
# End Group
# Begin Group "Misalignment"

# PROP Default_Filter ""
# Begin Source File

SOURCE=.\MainMisalign.c
# End Source File
# Begin Source File

SOURCE=.\MisalignNRPang.c
# End Source File
# End Group
# End Group
# Begin Group "Header Files"

# PROP Default_Filter "h;hpp;hxx;hm;inl"
# Begin Group "MonteCarlo Headers"

# PROP Default_Filter ""
# Begin Source File

SOURCE=.\FASTEXP2.H
# End Source File
# Begin Source File

SOURCE=.\RCONT2p.H
# End Source File
# Begin Source File

SOURCE=.\SUPPORT.H
# End Source File
# End Group
# Begin Source File

SOURCE=.\definitions.h
# End Source File
# Begin Source File

SOURCE=.\nrutilp.h
# End Source File
# Begin Source File

SOURCE=.\shevek.h
# End Source File
# End Group
# Begin Group "Resource Files"

# PROP Default_Filter "ico;cur;bmp;dlg;rc2;rct;bin;rgs;gif;jpg;jpeg;jpe"
# End Group
# End Target
# End Project
```

Shevek.dsw
Microsoft Developer Studio Workspace File, Format Version 6.00
WARNING: DO NOT EDIT OR DELETE THIS WORKSPACE FILE!

#####

Project: "shev"=".\\shev\\shev.dsp" - Package Owner=<4>

Package=<5>
{({
})}

Package=<4>
{({
})}

#####

Global:

Package=<5>
{({
})}

Package=<3>
{({
})}

#####

```

/*****
Written By Phillip S. Pang
*****/

```

```

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```

```

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*****/

```

```

/*****
STATEMENT OF COPYRIGHT
*****/

```

```

/*      Copyright 2001 by The Trustees of
/*      Columbia University in the City of
/*      New York. ALL RIGHTS RESERVED;
*/

```

```

/*****

```

```

/*****
/*****
/*****
/*
/*      Certain algorithms found within this file may be derivatives
/*      of source code obtained from the book:
/*      "Numerical Recipes in C: The Art of Scientific Computing"
/*      published by Cambridge University Press.
/*
/*****
/*****
/*****

```

```

/*****
/*****

```

```

/**      PROGRAM BEGINS      ***/

```

```

/*****
/*****

```

```

#include <string.h>
#include <stdio.h>
#include <stdlib.h>
#include <ctype.h>
#include <math.h>
#include <time.h>

```

```

#include "nrutilp.h"
#include "shevek.h"
#include "definitions.h"

```

```

double PRECISION;
int prec;

```

```

float  NUM_COL;
int    NUM_ROW;
int    OFFSET;

```

```

int    mainseq;
int    *dlength;

```

```

int    START;
int    STOP;

```

[illegible]

having to keep them*/

/*generates AR tables*/
/*outputs misalign.txt file*/

exitprogram();

free_cvector(input, 0, 0); /*frees memory allocated for */
/*aligned sequences */

}

/*
***** INTRO *****

*/

void intro()
{

int numread;
int numwrite;
char buf[10];
FILE *inputfile = NULL;

/* opens input file */

inputfile = fopen("titlepage", "r");

if (inputfile == NULL) printf("\nTITLE PAGE NOT FOUND\n");

else {

/*read FILE and writes to screen until end of file is reached*/

while(!feof(inputfile))
{
numread = fread(buf,sizeof(char),1,inputfile);
numwrite = fwrite(buf,sizeof(char),1,stdout);
}

fflush(inputfile);
fclose(inputfile);

}

}

/*
***** openfile *****

*/

char *openfile()
{

char *read_input(FILE *ifile);
char *input;
char filename[50];

extern int mainseq;
extern double PRECISION;
extern int prec;

extern int START;
extern int STOP;

FILE * inputfile = NULL;

int found_file = 0;

while (found_file == NO) { /*Queries for input file*/
printf("\nENTER alignment file name (include extension):");
scanf("%s", filename);
inputfile = fopen(filename, "r");
if (inputfile == NULL) {